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"Microwave & Infrared Observations of Molecular Spectra in Comet Kohoutek"

Funds were granted to assist with travel and other expenses connected with observations on Comet Kohoutek in both the microwave and the infrared regions.

Microwave measurements were made with a maser amplifier on the 80 ft. radio telescope of the Naval Research Laboratory in conjunction with personnel there. Nine transitions of possible molecules, H_2O, NH_3, CH_3OH, N_2O, and OH were searched for in Comet Kohoutek in the frequency range 22.2 - 25.2 GHz. These molecules were not detected, but upper limits for the optical depth, mean column density and production rate were derived for each of the molecules. In view of the reported detection of CH_3CH, the upper limits obtained for ammonia, for example, were surprisingly low. A detailed report of this work will be found in the accompanying manuscript, which has been submitted for publication in the journal ICARUS.

A search was made for the resonant scattering of solar infrared light at 5μ by CO molecules in Comet Kohoutek. Two observing periods were scheduled on the Lick 120 in. telescope in October and November, but unfortunately cloudy weather during both periods prevented any observations. Additional observation periods were scheduled on the 84 in. telescope at Mauna Kea. Again, there were some weather difficulties which, with logistic problems with equipment and cryogenic materials limited the observations. However, observations of moderate quality were obtained. These set an upper limit on the evolution of CO from Comet Kohoutek at about the level of expected rates. It is still quite low, however, in comparison with the reported rate of evolution for CH_3CN. A detailed description of these results is included in the accompanying manuscript which is also scheduled for publication in ICARUS.

MOLECULE SEARCHES IN COMET KOHOUTEK (1973f) AT MICROWAVE FREQUENCIES

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ABSTRACT

Nine transitions of the possible parent molecules H_2O, NH_3, CH_3OH and N_2O as well as the OH radical were searched for in Comet Kohoutek (1973f) in the frequency range 22.2-25.2 GHz. These molecules were not detected but the upper limits for the optical depth, mean column density and the production rate are derived for each of the molecules. These results are discussed and compared with the reported detections of HCN and CH_3CN emission and OH absorption.

The early discovery of the bright, young Comet Kohoutek (1973f) provided an excellent opportunity to search for several of the possible parent molecules (Huebner, 1970a, 1970b) evaporated from the icy nucleus of the comet near perihelion passage on December 28. During the period November 1973 - January 1974 we conducted a search for nine microwave transitions of five molecules--H_2O, NH_3, OH, CH_3OH, and N_2O. The searches yielded negative results.

The 85-foot (26m) reflector of the U. S. Naval Research Laboratory at Maryland Point Observatory was used for all observations. For the ammonia, methanol and nitrous oxide searches the receiver was equipped with a maser preamplifier ($T_{System} \sim 200°K$) developed at the University of California at Berkeley. For the water vapor, hydroxyl radical and some of the ammonia searches the receiver used a tunable parametric amplifier ($T_{System} \sim 850°K$) made available by the National Radio Astronomy Observatory.[1] Alternate back ends consisted of a bank of fifty 50 kHz contiguous filters and parallel banks of twenty-five 100 kHz and twenty 500 kHz filters with the same center frequency. At 24 GHz this corresponds to velocity resolutions of approximately 0.6, 1.2 and 6 km/sec respectively. Table I contains a summary of the observations.

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[1]The National Radio Astronomy Observatory is operated by Associate Universities, Incorporated, under contract with the National Science Foundation.

The nine transitions cover the frequency range 22.2-25.2 GHz. At these frequencies the antenna has a half-power beamwidth of ~ 2.2-2.0 arcmin, an aperture efficiency of approximately 0.4 and a main beam efficiency of approximately 0.5. An on-off technique with beam switching between comet and adjacent sky was used for all the data with typically 5-10 minute runs on source. An ephemeris for the topocentric position and velocity of the comet was generated at NRL using periodically updated orbital elements provided by B. G. Marsden (Smithsonian Astrophysical Observatory). The observations concentrated on the predicted positions for the comet nucleus but some of the searches included a grid around the predicted position and the extended tail of the comet.

Assuming the comet to be optically thin with a negligibly small optically thick center, the upper limit for the optical depth, τ, in terms of the observed peak-to-peak antenna temperature, T_A, is

$$T_A = \eta_B B(T-T_b)\ (1-e^{-\tau}) = \eta_B B(T-T_b)\tau \qquad (1)$$

where η_B = main beam efficiency, B = beam dilution factor, T_b = 2.7°K microwave background continuum and T = temperature of cometary gas. A value of T = 200°K was assumed for the evaluation of the upper limits. This value is consistent with the 200°K equilibrium temperature of a water clathrate model for the comet at a heliocentric distance of R = 1 A.U. (Jackson, 1972).

The optical depths at the center of a Doppler-broadened line for the linear molecules N_2O and OH, the symmetric top

NH_3 and the asymmetric tops H_2O and CH_3OH were taken to be respectively (Huebner, 1970b),

$$\tau = \frac{4\ \pi^{5/2}\ \ hf_v}{3ck^2}\ \frac{\mu^2\ \nu^3}{T^3\ \Delta\nu}\ e^{-W/kT}\ N$$

$$\tau = \frac{16\ \pi^2 h^{3/2} f_v}{3ck^{5/2}}\ \frac{B\sqrt{C}\ \mu^2\ \nu^2}{T^{5/2}\ \Delta\nu}\ \frac{(2J+1)\ K^2}{J\ (J+1)}\ e^{-W/kT}\ N.$$

$$\tau = \frac{8\ \pi^2 h^{3/2}\ f_v}{3ck^{5/2}}\ \frac{\sqrt{ABC}\ \mu^2\ \nu^2}{T^{5/2}\ \Delta\nu}\ S\ e^{-W/kT}\ N \tag{2}$$

where all quantities are in cgs units, h = Planck's constant, k = Boltzmann's constant, c = light velocity, $f_v = 1$ for transitions considered, all in ground vibrational level, ν = frequency (Hz), μ = dipole moment (esu-cm), T = cometary gas temperature (°K), $\Delta\nu$ = line half-width at e^{-1} of maximum intensity (Hz), A,B,C are rotational constants (Hz); $A \geq B \geq C$, J and K are quantum numbers of upper rotational sate, W = energy of upper rotational state, S = line strength of transition and N = column density of molecular species considered in cm^{-2}.

The beam dilution was taken into account in the usual way using the optical depth averaged over the antenna beam $\langle\tau\rangle = B\,\tau$ in Eq. (1) and the column density derived from Eq. (2) is then the uniformly smeared out or averaged column density of the molecules in all states in the antenna beam $\langle N \rangle$ (Huebner and Snyder, 1970). Table II contains the results for the upper limits of the average optical depths and column densities.

Since the velocity of the possible parent molecules such as H_2O, NH_3, CH_3OH and N_2O is determined by the equilibrium

temperature with the icy neculeus (Jackson, 1972) the linewidths were calculated from the expression for the Doppler half-width at e^{-1} of maximum intensity $\Delta \nu = \nu \sqrt{2kN_oT/M}\ /C$ where $T = 200°K$, M = molecular weight and N_o = Avogadro's number. The full-width at half-intensity $2\ (\ln 2)^{1/2}\ \Delta \nu$ for these molecules would be 38-58 kHz. The Doppler width was also used for the OH radical upper limits, however, the velocity of OH depends upon the actual radical production mechanism (Jackson, 1972). OH line widths of about 2 km/sec may have to be considered (Turner, 1974).

Upper limits for the molecule production rate Q in molecules/sec/steradian were estimated from its relation to the average column density $\langle N \rangle$ (Huebner and Snyder, 1970).

$$Q = \frac{v\ \Delta^2\ \theta^2}{16}\ [s\ \cos^{-1} \frac{s}{r_o} - (r_o^2 - s^2)^{1/2} + r_o]^{-1}\ \langle N \rangle \qquad (3)$$

where v is the average expansion velocity of the molecular species which is approximately 0.3-0.4 km/sec, r_o = destruction radius for the molecule where $r_o = v\ \tau_o$ with τ_o the lifetime of the molecules, Δ = geocentric distance of comet, θ = full width of antenna beam at half power and s is the smaller of the two quantities r_o and $\Delta\ (\theta/2)$. Typically, $\Delta\ (\theta/2) = 4\text{-}5 \times 10^4$ km. At a heliocentric distance of 1 A.U. the parent molecules have lifetimes against photodissociation on the order of 10^4-10^5 sec (Jackson, 1974). Values of the molecular yield Q (molecules/sec/ster) estimated for the typical values $r_o = 10^4$ and 10^5 km are contained in Table III.

An estimate for the molecular yield of OH can be made if one considers that the OH radical is in an extended cloud

around the nucleus with an $r_o \sim 10^6$ km at R = 1 A.U. (Delsemme, 1973), or $r_o \sim 6 \times 10^5$ km at R = 0.8 A.U. appropriate for our OH observations. In this case the OH filled the beam and the upper limit of $\langle N \rangle < 4.2 \times 10^{16}$ cm^{-2} yields a value of $Q < 2 \times 10^{31}$ OH radicals produced/sec/steradian. Turner (1974) has reported the detection of the 1665 and 1667 MHz lines of OH in Comet Kohoutek in absorption against a 3°K background. He derived a value of $N = 6 \times 10^{14}$ cm^{-2} in the ground state with a beamwidth of 18 arcmin and estimates the size of the OH halo to be about 11 arcmin in early December which corresponds to $r_o \sim 4 \times 10^5$ km in agreement with the value used above.

Huebner, Snyder and Buhl (1974) have detected HCN in Comet Kohoutek with estimates for the HCN production rate of $Q \sim 2\text{-}7 \times 10^{26}$ molecules/sec/steradian. If the production rates for the molecules of Table III are actually similar to that of HCN then our upper limits for Q are not very stringent except for the case of NH_3 whose production rate might be comparable to HCN. Our non-detection of NH_3 may have been due to a smaller destruction radius or to a relatively lower initial abundance within the icy nucleus. The contrast is more striking when one compares NH_3 with CH_3CN. Ulich and Conklin (1974) have reported the detection of two vibrationally excited rotational transitions of methyl cyanide, CH_3CN in Comet Kohoutek with an estimated column density of $N = 3 \times 10^{16}$ cm^{-2} in early December. For the beam dilution used (B = .06)

this would correspond to $\langle N \rangle = BN = 2 \times 10^{15}$ cm^{-2}. For typical values of the destruction radius, $r_o = 10^4$ km, this would be equivalent to a production rate of $\dot{Q} = 2 \times 10^{29}$ CH_3CN molecules/sec/steradian while for $r_o = 10^5$ km, the rate would be $Q = 4 \times 10^{28}$. Our upper limit indicates that CH_3OH was produced at a slower rate than the detected CH_3CN but the production rate of CH_3OH could have been comparable to that of the detected HCN.

The temperatures required to produce 1 mm of gas pressure for N_2O, NH_3, HCN, CH_3CN, CH_3OH and H_2O are respectively 130°, 164°, 202°, 226°, 229° and 266°K (Handbook of Chemistry and Physics, 1967-1968). The two molecules detected are among the least volatile on this list. Our upper limits set for the abundances of N_2O, CH_3OH and H_2O are sufficiently large to perhaps not be very significant. Indeed, the presence of H_2O in the cometary gas is inferred by Wehinger et al. (1974) who detected the H_2O^+ ion in the comet tail. However, the low abundance of NH_3 is surprising and may be due to its having been lost by evaporation during some past history of the comet or to formation of the comet at temperatures which were too high to condense much NH_3 in the nucleus.

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TABLE I

MOLECULE SEARCHES IN COMET KOHOUTEK (1973f)

Molecule	Transition	Rest Frequency MHz	Observation Dates 1973-1974	Δ(AU)[1]	Filter Resolution kHz	Receiver[2]	Integration Time (minutes)
H_2O	6_{16}-5_{23}	22235.08	Nov 14, Jan 2,18	0.9	50	P	120
H_2O	6_{16}-5_{23}	22235.08	Nov 14, 16, 26	1.6	100,500	P	140
NH_3	(1,1)	23694.49	Dec 22	1.1	50	M	85
NH_3	(1,1)	23694.49	Nov 23	1.5	100,500	P	90
NH_3	(2,2)	23722.63	Nov 23	1.5	100,500	P	20
NH_3	(3,3)	23870.13	Dec 16, 20, 23	1.0	50	M	140
NH_3	(3,3)	23870.13	Nov 19	1.6	100,500	P	40
OH	J=9/2,F=4-4	23818.18	Jan 18, 22	0.8	50	P	80
OH	J=9/2,F=4-4	23818.18	Jan 22	0.8	100,500	P	30
OH	J=9/2,F=5-5	23826.90	Jan 23	0.8	50	P	70
OH	J=9/2,F=5-5	23826.90	Jan 23	0.8	100,500	P	30
OH (Comet Tail)	J=9/2,F=5-5	23826.90	Jan 23	0.8	50	P	40
CH_3OH	7_2-7_1(E)	25124.88	Dec 13, 14, 15, Jan 5	1.2	50	M	135
CH_3OH	2_2-2_1(E)	24934.38	Dec 12	1.2	50	M	20
N_2O	1-0	25123.25	Dec 13, Jan 5	1.0	50	M	30

[1] Average geocentric distance of comet in A.U.

[2] M = maser preamplifier, P = tunable parametric amplifier

TABLE II

UPPER LIMITS FOR MOLECULE SEARCHES IN COMET KOHOUTEK (1973f)

Molecule	Transition	F/R[1]	Peak-to-Peak T_A(°K)	Upper Limit ⟨τ⟩	Upper Limit (cm^{-2}) ⟨N⟩
H_2O	$6_{16} - 5_{23}$	50 P	0.80	.0060	5.0×10^{16}
NH_3	(1,1)	50 M	0.25	.0024	5.4×10^{13}
NH_3	(2,2)	100 P	4.07	.0400	5.0×10^{14}
NH_3	(3,3)	50 M	0.28	.0027	1.5×10^{13}
OH	J=9/2,F=4-4	50 P	1.35	.0133	6.2×10^{16}
OH	J=9/2,F=5-5	50 P	0.92	.0104	4.2×10^{16}
OH (Tail)	J=9/2,F=5-5	50 P	1.75	.0170	8.0×10^{16}
CH_3OH	$7_2 - 7_1$(E)	50 M	0.32	.0032	9.0×10^{14}
CH_3OH	$2_2 - 2_1$(E)	50 M	0.91	.0092	8.4×10^{15}
N_2O	1 - 0	50 M	1.89	.0194	1.5×10^{17}

[1]F/R denotes filter resolution in kHz/receiver, where M = maser preamplifier and P = tunable parametric amplifier

TABLE III

UPPER LIMITS FOR MEAN COLUMN DENSITY AND MOLECULE PRODUCTION RATE

COMET KOHOUTEK (1973f)

Molecule	⟨ N ⟩	Q	
		$r_o = 10^4$ km	$r_o = 10^5$ km
H_2O	5×10^{16}	1×10^{31}	2×10^{30}
NH_3	1.5×10^{13}	4×10^{27}	6×10^{26}
CH_3OH	9×10^{14}	1×10^{29}	2×10^{28}
N_2O	1.5×10^{17}	2×10^{31}	3×10^{30}

⟨ N ⟩ = upper limit for mean column density uniformly spread out over antenna beam (molecules-cm^{-2}) where the number of molecules refers to the total number of molecules in all states

Q = upper limit for molecule production rate (molecules-sec^{-1}-steradian^{-1})

AN UPPER LIMIT ON THE EVOLUTION OF CARBON MONOXIDE FROM COMET KOHOUTEK *

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UPPER LIMIT ON CO IN COMET KOHOUTEK

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ABSTRACT

An upper limit on the rate of evolution of CO from Comet Kohoutek has been obtained from a search for resonant scattering of sunlight near 4.7μ. The observations were made approximately two months after perihelion. The rate of evolution of CO at that time was apparently less than that of CH_3CN observed before perihelion.

Under favorable conditions, and with a very sensitive spectrometer, infrared resonant scattering of sunlight should allow a determination of the rate of evolution of CO from a bright comet (Biermann, 1973a). Such a determination was attempted for Comet Kohoutek 1973f. Optimum observing conditions were not obtained and CO not detected, but the limited measurements which could be made provide an upper limit on the CO evolution rate approximately two months after perihelion.

Observations were made on February 23, 1974 at the Mauna Kea Observatory's 88" telescope using a tandem scanning Fabry-Perot interferometer (Holtz, 1971). The field of view was 9.5" by 14" and was approximately centered on the comet's nucleus. A spectral region near 4.7μ including the 1-0 P2 and P3 fundamental rotation-vibration transitions of $^{12}C^{16}O$ was scanned with a resolution of 0.1 cm^{-1}. The comet's radial velocity of 47 km s^{-1} with respect to the earth, giving a doppler shift of 0.33 cm^{-1}, was sufficient to move the expected positions of the cometary lines well outside the half-power points of the terrestrial CO line absorption.

The sensitivity of the spectrometer system was determined by measurement of the signal from W Hya in the same wavelength region. If σ represents the r.m.s. noise fluctuation, any signal larger than 3σ should have been easily observed. With this criterion, the lack of an observed signal sets an upper

limit of 1.0×10^{-18} W cm^{-2} for the flux in either CO line at the top of the earth's atmosphere. Since the rate of resonant scattering of 4.7μ radiation by a CO molecule at 1.5 A.U. from the sun is approximately 6×10^{-5} s^{-1}, the above limit for the flux corresponds to an upper limit of 2.5×10^{33} for the total number of CO molecules within the field of view in a single rotation-vibration state. For an assumed temperature of 250° K, the J=3 level contains about 7% of all CO molecules present. Thus, the upper limit on the total amount of CO in the field of view is 3.5×10^{34}.

Assuming a model in which CO is produced in a region small compared to the observed field of view, the density of CO is given by $n(CO) = \frac{4Q}{\pi\bar{v}} \cdot \frac{1}{r^2}$; where $4\pi Q$ is the total production rate, r the distance from the source, and $\bar{v}$ is the mean speed $\sqrt{\frac{8kT}{\pi m}}$. For a molecular lifetime τ, the CO cloud will have a radius $r_o = \bar{v}\tau$. The total number of molecules within a circular field of radius ρ centered on the comet is approximately $2(\frac{4\pi Q}{\bar{v}})\,\rho$ if $\rho < r_o$, which is almost certainly the case. At a distance of 1.5 A.U., the rectangular field of view has the area of a circular field of radius $\rho = 7.3 \times 10^8$ cm. Hence the observed limit on the flux corresponds to $Q/\bar{v}$ (CO) $< 2 \times 10^{24}$ cm^{-1} $ster^{-1}$. Biermann (1973a) has estimated that $Q/\bar{v}$ for CO in bright comets is $10^{23\pm1}$.

Ulich and Conklin (1974) have reported a detection of CH_3CN in Comet Kohoutek by its microwave emission and concluded that the total number of methyl cyanide molecules within their antenna beam was ~9 x 10^{34}. The observations were made in early December, before perihelion. They estimate the CH_3CN cloud radius to be ~10^9cm, which is considerably smaller than the size of the microwave antenna beam. In that case,

$$Q/\bar{v}\ (CH_3CN) = \frac{N}{4\pi\ \rho_{cloud}} = 7.2 \times 10^{24}\ cm^{-1}\ ster^{-1}$$

If the CH_3CN cloud is larger than the estimated 10^9cm, a lower limit on $Q/\bar{v}$ is given by $\frac{N}{4\pi\ \rho_{beam}}$. The effective radius of the beam used by Ulich and Conklin is ~4 x 10^9cm, so that

$$Q/\bar{v}\ (CH_3CN) > 1.8 \times 10^{24}\ cm^{-1}\ ster^{-1}$$

This is essentially equal to the above upper limit for CO,

$$Q/\bar{v}\ (CO) < 2 \times 10^{24}\ cm^{-1}\ ster^{-1}$$

It is surprising that the rate of evolution from the comet reported for CH_3CN is equal to or greater than the rate of evolution of CO. However, it must be noted that CH_3CN was detected before perihelion when the comet was approximately 0.8 A.U. from the sun. Subsequent search after perihelion failed to detect this molecule. Observations which set the present upper limit on CO were made only after perihelion, when the comet was ~1.5 A.U. from the sun. Since one would expect the

rate of evolution of CO to be much greater than that of CH_3CN, it is unlikely that this difference in heliocentric distance can account for the apparent abundances. It is more likely that the comet lost most of its volatile gases such as CO in the course of its trajectory before and during perihelion, (cf. Biermann, 1973b) or that the more volatile gases were already depleted long before its recent approach to the sun.

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SYMBOLS

μ	lower case Greek mu
σ	lower case Greek sigma
π	lower case Greek pi
( )"	arc seconds (as 9.5" by 14") or inches (as 88")
<	less than
>	greater than
~	approximately equal to
$\bar{v}$	lower case Arabic v with bar